201-14960

HIGH PRODUCTION VOLUME (HPV) CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For

Eicosenoic acid, methyl ester, (Z)-

CAS No. 76899-35-9

Submitted to the US EPA

BY

Crompton Corporation.

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Test Plan for Eicosenoic acid, methyl ester, (Z)-

1. General Information

1.1 CAS Number: 76899-35-9

1.2 Molecular Weight: 324.55

1.3 Structure and formula: $C_{21}H_{40}O_2$

$H_3CO_2C(CH_2)_8CHCH(CH_2)_8CH_3$

1.4 Introduction

The substance is used as ??????????

2. Review of Existing Data and Development of Test Plan

Crompton Corporation has undertaken a comprehensive evaluation of all relevant data on the SIDS endpoints of concern for the substance.

The availability of the data on the specific SIDS endpoints is summarized in Table 1. Table 1 also shows data gaps that will be filled by additional testing.

Table 1: Available adequate data and proposed testing on eicosenoic acid, methyl ester, (Z)-

CAS No. 76899-35-9	Information Available?	GLP	OECD Study?	Other Study?	Estimation Method?	Acceptable?	SIDS Testing required?
	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
Physicochemical							
Melting Point	Y				Y	Y	N
Boiling Point	Y				Y	Y	N
Vapour Pressure	Y				Y	Y	N
Water Solubility	Y				Y	Y	N
Partition Coefficient (Kow)	Y				Y	Y	N
Environmental Fate							
Biodegradation	Y				Y	Y	N
Hydrolysis	Y				Y	Y	N
Photodegradation	Y				Y	Y	N
Transport and Distribution between Environmental Compartments	Y				Y	Y	N
Ecotoxicology							
Acute Fish	Y				Y	Y	N
Acute Daphnia	Y				Y	Y	N
Acute Algae	Y				Y	Y	N

Toxicology							
Acute Oral	N						Y
Repeat Dose toxicity	N						Y
Genetic toxicity – Gene mutation	N						Y
Genetic toxicity – Chromosome aberration	N						Y
Reproductive toxicity	N						Y
Developmental toxicity/teratogenicity	N						Y

A. Evaluation of Existing Physicochemical Data and Proposed Testing

1. Melting Point

The melting point was estimated to be 98.13°C using MPBPWIN v 1.40.

2. Boiling Point

The boiling point was estimated to be 375.8°C using MPBPWIN v 1.40.

3. Vapor Pressure

The vapor pressure was estimated to be 0.0000083 hPa at 25°C using MPBPWIN v 1.40.

4. Water Solubility

The water solubility is estimated to be 0.00018 mg/L at 25°C using WSKOW v 1.40.

5. Partition Coefficient

The Log Pow is estimated to be 9 using KOWWIN v 1.66.

Summary of Physicochemical Properties Testing: Existing data for melting point, boiling point, vapour pressure, partition coefficient and water solubility are considered to fill these endpoints adequately.

B. Evaluation of Existing Environmental Fate Data and Proposed Testing

1. Biodegradation

The biodegradability of the chemical has been estimated using Biowin v4.00 and the results indicate the chemical to be readily biodegradable.

2. Hydrolysis

The half life at pH 7 is estimated to be 7.28 years, and at pH 8 266 days using HYDROWIN v 1.67.

3. Photodegradation

The potential for photodegradation of the chemical has been estimated using the AOPWIN v1.90, and indicated atmospheric oxidation via OH radicals reaction with a half-life of 1.5 – 1.65 hours (cis- & trans- isomers, respectively).

4. Transport and Distribution between Environmental Compartments

An Epiwin Level III Fugacity Model calculation has been conducted and indicates distribution mainly to sediment and, to a lesser extent, soil for emissions of 1000 kg/hr simultaneously to air water and soil compartments.

Summary of Environmental Fate Testing: Existing data for photodegradation, biodegradation, hydrolysis and transport and distribution between environmental compartments are considered to fill these endpoints adequately.

C. Evaluation of Existing Ecotoxicity Data and Proposed Testing

1. Acute Toxicity to Fish

The LC_{50} (96 h) was estimated to be 0.009 mg/L using ECOSAR v 0.99g. This is greater than the estimated limit of solubility of the substance.

2. Acute Toxicity to Daphnia

The EC_{50} (48 h) was estimated to be 0.00011 mg/L using ECOSAR v 0.99g.

3. Acute Toxicity to Algae

The EC_{50} (96 h) was estimated to be 0.0009 mg/L using ECOSAR v 0.99g. This is greater than the estimated limit of solubility of the substance.

Summary of Ecotoxicity Testing: The substance is estimated to be readily biodegradable and toxic to the aquatic environment close to, or above its limit of solubility. No further testing is proposed.

D. Evaluation of Existing Human Health Effects Data and Proposed Testing

1. Acute Oral Toxicity

An OECD 423 study will be conducted to fill this endpoint.

2. Repeat Dose Toxicity

An OECD 422 study will be conducted to fill this endpoint.

3. Genotoxicity

OECD 471 and 473 studies will be conducted to fill this endpoint.

4. Reproductive and Developmental Toxicity

An OECD 422 study will be conducted to fill this endpoint.

Summary of Human Health Effects Testing: No data exists for the human health effects endpoints. Appropriate studies will be conducted to fill these endpoints.

3. Evaluation of Data for Quality and Acceptability

The collected data were reviewed for quality and acceptability following the general US EPA guidance [2] and the systematic approach described by Klimisch et al [3]. These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. This scoring system was only applied to ecotoxicology and human health endpoint studies per EPA recommendation [4]. The codification described by Klimisch specifies four categories of reliability for describing data adequacy. These are:

(1) Reliable without restriction: Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.

(2) Reliable with Restrictions: Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.

(3) Not Reliable: Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.

(4) Not Assignable: Includes studies or data in which insufficient detail is reported to assign a rating, e.g. listed in abstracts or secondary literature.

4. References

[1] US EPA, EPI Suite Software, 2000

[2] USEPA (1998). Guidance for Meeting the SIDS Requirements (The SIDS Guide). Guidance for the HPV Challenge Program. Dated 11/2/98.

[3] Klimisch, H.-J., et al (1997). A Systematic Approach for Evaluating the Quality of Experimental Toxicological and Ecotoxicological Data. Regul. Toxicol. Pharmacol. 25:1-5

[4] USEPA (1999). Determining the Adequacy of Existing Data. Guidance for the HPV Challenge Program. Draft dated 2/10/99.